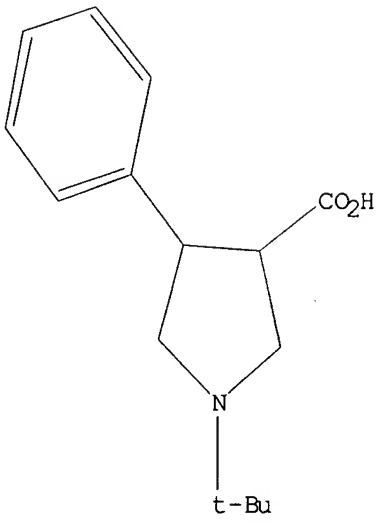
STN structure search (Registry / Caplus)



G1 H,MeO

Structure attributes must be viewed using STN Express query preparation.

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=> s l1
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SAMPLE SCREEN SEARCH COMPLETED -       47 TO ITERATE

100.0% PROCESSED       47 ITERATIONS                          0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:          529 TO     1351
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 15:56:30 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      994 TO ITERATE

100.0% PROCESSED      994 ITERATIONS                          8 ANSWERS
SEARCH TIME: 00.00.01

L3            8 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             172.10     172.31

FILE 'CAPLUS' ENTERED AT 15:56:36 ON 30 MAY 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 30 May 2007 VOL 146 ISS 23
FILE LAST UPDATED: 29 May 2007 (20070529/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l3
L4 14 L3

=> d ibib abs hitstr 1-14

L4 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:410486 CAPLUS
DOCUMENT NUMBER: 146:421856
TITLE: Acylated spiropiperidine derivatives as melanocortin-4 receptor modulators and their preparation, pharmaceutical compositions and use in the treatment of diseases
INVENTOR(S): Jian, Tianying; Liu, Jian; Nargund, Ravi P.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 159pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007041052	A2	20070412	WO 2006-US37196	20060925

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2005-721678P P 20050929

GI

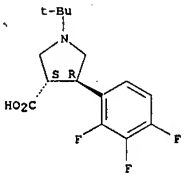
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Certain N-acylated spiropiperidine derivs. of formula I are ligands of the human melanocortin receptor(s) and, in particular, are selective ligands of the human melanocortin-4 receptor (MC-4R). They are therefore useful for the treatment, control, or prevention of diseases and disorders responsive to the modulation of MC-4R, such as obesity, diabetes, nicotine addiction, alcoholism, sexual dysfunction, including erectile dysfunction and female sexual dysfunction. Compds. of formula I wherein A is (un)substituted heteroaryl; X and Y taken together to form CR6=CR6; one of X and Y is CR62 and the other is CR62, NR6, CO C=NR6, C=CR62, O, S, SO and SO2; one of X and Y is NR9, and the other is CR62, CO, C=NR6, C=CR62, SO and SO2; one of X and Y is CO and the other is CR62, NR6, C=NR6, O and S; Z is CH and N, provided that when Z is N, R1 is not NH2 and derivs.; R1 is H, (alkyl)amine, amidino, C1-6 alkyl, (hetero)aroyl, (alkyl)(hetero)aryl, etc.; R2 is Ph, naphthyl and heteroaryl; R6 is H, C1-6 alkyl, (alkyl)(hetero)aryl, alkoxyalkyl, cyanoalkyl, etc.; R9 is H, C1-6 alkyl, (alkyl)heteroaryl, (alkyl)-C3-7 cycloalkyl, alkylcarboxylic acid derivs., etc.; R11 is H, OH, C1-8 alkyl, O-C1-8 alkyl, halo, NH and derivs., SH and derivs., and CF3; m and n are independently 1 and 2; and their pharmaceutically acceptable salts thereof, are claimed. Example compd. II was prepd. by a multistep procedure (procedure given). All the invention compds. were evaluated for their melanocortin-4 receptor modulatory activity. The tested compds. were found to bind to melanocortin-4 receptor with IC50 values less than 10 μM.

IT 934361-22-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of acylated spiropiperidine derivs. as melanocortin-4 receptor modulators)

RN 934361-22-5 CAPLUS
CN 3-Pyrrolidinecarboxylic acid, 1-(1,1-dimethylethyl)-4-(2,3,4-trifluorophenyl)-, (3S,4R)- (CA INDEX NAME)

Absolute stereochemistry.

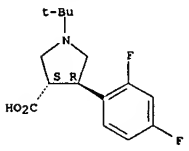


IT 455957-94-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of acylated spiropiperidine derivs. as melanocortin-4 receptor modulators)

RN 455957-94-5 CAPLUS
CN 3-Pyrrolidinecarboxylic acid, 4-(2,4-difluorophenyl)-1-(1,1-dimethylethyl)-, (3S,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L4 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



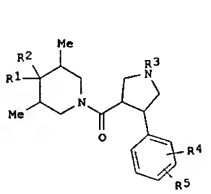
L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:150961 CAPLUS
DOCUMENT NUMBER: 146:229190
TITLE: Preparation of pyrrolidinylcarbonylpiperidines as melanocortin subtype 4 (MC4) receptor agonists for treatment of lower urinary tract dysfunction.
INVENTOR(S): McMurray, Gordon; Phillips, Stephen Charles; Westbrook, Simon Lempriere
PATENT ASSIGNEE(S): Pfizer Limited, UK
SOURCE: PCT Int. Appl., 85pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007015157	A2	20070208	WO 2006-IB2119	20060720

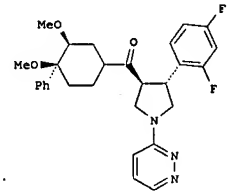
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: GB 2005-15817 A 20050801
US 2005-705237P P 20050802

OTHER SOURCE(S): MARPAT 146:229190
GI



I

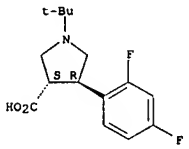


II

AB Use of MC4 receptor antagonists, e.g. [I; R1 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, aryl, heterocyclyl, etc.; R2

L4 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
H, OH, OMe; R3 = H, Rl; R4, R5 = H, halo, alkyl, alkenyl, alkynyl, cyano, CF3, CH2CF3, OCF3, OCH2CF3, cycloalkenyl(alkyl), amino(alkyl), etc.; R4R5 = atoms to form fused 5-7 membered (unsatd.) ring] for the manuf. of a medicament for the treatment of lower urinary tract dysfunction is claimed. Thus, title compd. (II) (prepn. outlined) at 2 mg/kg i.v. in the dog urethral pressure model gave a 20% increase in peak urethral pressure.
IT 455957-94-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrrolidinylcarbonylpiperidines as MC4 receptor agonists for treatment of lower urinary tract dysfunction)
RN 455957-94-5 CAPLUS
CN 3-Pyrrolidinecarboxylic acid, 4-(2,4-difluorophenyl)-1-(1,1-dimethylethyl)-, (3S,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L4 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:150182 CAPLUS
DOCUMENT NUMBER: 146:229186
TITLE: Preparation of piperidinoyl-pyrrolidine and piperidinoyl-piperidine compounds as MCR4 agonists
INVENTOR(S): Andrews, Mark David; Brown, Alan Daniel; Fradet, David
Sebastien; Lansdell, Mark Ian
PATENT ASSIGNEE(S): Pfizer Limited, UK
SOURCE: PCT Int. Appl., 103pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007015162	A1	20070208	WO 2006-IB2151	20060726

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2005-706191P P 20050804

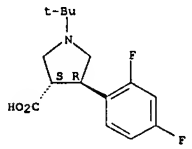
OTHER SOURCE(S): MARPAT 146:229186
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [n = 1, 2; R6 = H, alkyl, cycloalkyl, etc.; R7 = pyridinyl or Ph (wherein pyridinyl or Ph is optionally substituted by halo, CN, CF3, etc.); R10 = Q1; R1, R4 = H, alkyl, OH, etc.; R2 = H, OH, O-alkyl, etc.; R3 = aryl or heteroaryl (wherein said moieties are optionally substituted by halo, CN, CF3, etc.); R5 = H or alkyl; R1, R4 and R5 are not all simultaneously H.; when R1 is Me and R4 is H, then R5 is not Me.; when R4 is Me and R5 is H, then R1 is not Me.; when R5 is Me and R4 is H, then R1 is not Me.), pharmaceutically acceptable salts, hydrates, solvates, polymorphs, and prodrugs thereof were prepared For example, amidation of (3S,4R)-1-tert-butyl-4-(2,4-difluorophenyl)pyrrolidine-3-carboxylic acid hydrochloride, e.g., prepared from (E)-2,4-difluorocinnamic acid in 3 steps, with (3S,4R)-3-methyl-4-phenylpiperidin-4-ol followed by treatment with

L4 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
HCl afforded compd. II·HCl. Compds. according to the invention herein exhibited a binding const. at the MCR4 (melanocortin receptor 4) expressed as an Ki value against AGRP (agouti related protein) lower than 1000 nM. Compds. I are claimed useful for the treatment of sexual dysfunction and obesity.
IT 455957-75-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of piperidinoyl-pyrrolidine and piperidinoyl-piperidine compds. as MCR4 agonists)
RN 455957-75-2 CAPLUS
CN 3-Pyrrolidinecarboxylic acid, 4-(2,4-difluorophenyl)-1-(1,1-dimethylethyl)-, hydrochloride (1:1), (3S,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



● HCl

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

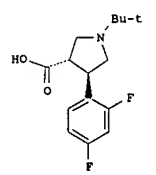
L4 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:14419 CAPLUS
DOCUMENT NUMBER: 146:121832
TITLE: Preparation of pyrrolidinylcarbonylpiperidine derivative as MC4R agonist and of crystalline forms of said derivative
INVENTOR(S): Calabria, Ralph; Cheng, Yu; Ferlita, Russell R.; Kamali, Ashkan; Murry, Jerry A.; Mathre, David; Peresypkin, Andrey V.; Thompson, Karen; Wang, Jian; Wenslow, Robert M.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 50pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007002462	A2	20070104	WO 2006-US24573	20060623

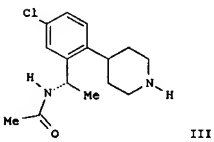
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2005-694488P P 20050627

GI



II

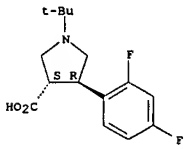


III

AB The present invention relates to a process for producing N-((1S)-1-[2-(1-{[(3S,4R)-1-tert-butyl-4-(2,4-difluorophenyl)pyrrolidin-3-yl]carbonyl}piperidin-4-yl)-5-chlorophenyl]ethyl}acetamide (I), and novel

L4 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
cryst. salts, hydrates, solvates, and polymorphic forms thereof. Thus, treatment of pyrrolidinecarboxylic acid II with CDI in acetonitrile, followed by reaction with piperidine deriv. III in acetonitrile in the presence of triethylamine gave, after workup, I (free base). A soln. of I
(free base) in iso-Pr acetate was mixed with 0.5 N HCl/H2O soln. to give, after workup and crystn., the cryst. hydrate mono-HCl salt of I.
IT 455957-94-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrrolidinylcarbonylpiperidine derivative as MC4R agonist and of
crystalline forms of said derivative)
RN 455957-94-5 CAPLUS
CN 3-Pyrrolidinecarboxylic acid, 4-(2,4-difluorophenyl)-1-(1,1-dimethylethyl)-, (3S,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L4 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:165649 CAPLUS
DOCUMENT NUMBER: 144:232924
TITLE: Preparation of piperidine derivatives as melanocortin-4 receptor agonists
INVENTOR(S): Barakat, Khaled J.; Guo, Liangqin; Liu, Jian; Nargund, Ravi P.; Sebhat, Iyassu K.; Ye, Zhixiong
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 79 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006019787	A2	20060223	WO 2005-US24806	20050713
WO 2006019787	A3	20060914		
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RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
AU 2005275232	A1	20060223	AU 2005-275232	20050713
CA 2573714	A1	20060223	CA 2005-2573714	20050713
EP 1773347	A2	20070418	EP 2005-769526	20050713
PRIORITY APPLN. INFO.:			US 2004-588494P P	20040716
			WO 2005-US24806 W	20050713

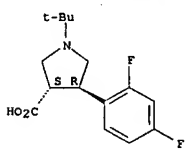
OTHER SOURCE(S): MARPAT 144:232924
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title piperidine derivs. I [wherein m = 0-2; n = 1-2; R1 and R2 = independently halo, CF3, CH3, and OMe; R3 and R4 = independently halo, CF3, CN, alkyl, alkoxy, etc.; R5 = OH, halo, alkyl, alkoxy, etc.], or pharmaceutically acceptable salts thereof were prepared as agonists of the human melanocortin-4 receptors (MCR-4). For example, II was prepared in a multi-step synthesis. The title compds. showed IC50 less than 10 μM against MCR-4. Formulations with finely divided lactose as hard gelatin

L4 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
capsule have been described. The compds. are useful for the treatment, control, or prevention of diseases and disorders responsive to the activation of MCR-4, such as obesity, diabetes, male or female sexual dysfunction.
IT 455957-94-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of piperidine derivs. as MCR-4 agonists)
RN 455957-94-5 CAPLUS
CN 3-Pyrrolidinecarboxylic acid, 4-(2,4-difluorophenyl)-1-(1,1-dimethylethyl)-, (3S,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

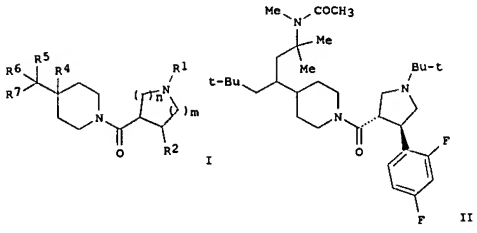


L4 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:164650 CAPLUS
DOCUMENT NUMBER: 144:254006
TITLE: Preparation of piperidine derivatives as melanocortin-4 receptor agonists
INVENTOR(S): Bakshi, Raman K.; Dellureficio, James P.; Nargund, Ravi P.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 78 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006020277	A2	20060223	WO 2005-US25505	20050715
WO 2006020277	A3	20060720		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
AU 2005274701	A1	20060223	AU 2005-274701	20050715
CA 2574156	A1	20060223	CA 2005-2574156	20050715
EP 1773338	A2	20070418	EP 2005-773009	20050715
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR				
PRIORITY APPLN. INFO.:			US 2004-589089P P	20040719
			WO 2005-US25505 W	20050715

OTHER SOURCE(S): MARPAT 144:254006
GI

L4 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



I II

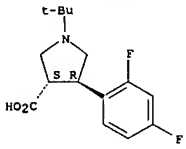
AB The title piperidine derivs. I [wherein m = 0-2; n = 1-2; R1 = H, amidino, alkyl, etc.; R2 = (un)substituted Ph, naphthyl, or heteroaryl; R4 = H, alkyl, alkoxy, etc.; R5 = CF3, alkyl, alkenyl, alkynyl, etc.; R6 = H, alkyl, or alkoxy; R7 = NH2, CN, OH, alkoxy, etc.], or pharmaceutically acceptable salts thereof were prepared as agonists of the human melanocortin-4 receptors (MCR-4). For example, II was prepared in a multi-step synthesis. The title compds. showed IC50 less than 10 μM against MCR-4. Formulations with finely divided lactose as hard gelatin capsule have been described. The compds. are useful for the treatment, control, or prevention of diseases and disorders responsive to the activation of MCR-4, such as obesity, diabetes, male or female sexual dysfunction (no data).

IT 455957-94-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of piperidine derivs. as MCR-4 agonists)

RN 455957-94-5 CAPLUS

CN 3-Pyrrolidinecarboxylic acid, 4-(2,4-difluorophenyl)-1-(1,1-dimethylethyl)-, (3S,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



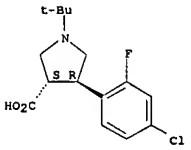
L4 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

IT 757974-04-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of piperidine derivs. as MCR-4 agonists)

RN 757974-04-2 CAPLUS

CN 3-Pyrrolidinecarboxylic acid, 4-(4-chloro-2-fluorophenyl)-1-(1,1-dimethylethyl)-, (3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:735328 CAPLUS
DOCUMENT NUMBER: 143:211844
TITLE: Preparation of Pyrrolidinyl(carbonyl) piperidines as melanocortin receptor 4 agonists for therapeutic use
INVENTOR(S): Calabrese, Andrew Antony; Fradet, David Sebastien; Hepworth, David; Lansdell, Mark
PATENT ASSIGNEE(S): Pfizer Inc, UK
SOURCE: U.S. Pat. Appl. Publ., 102 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

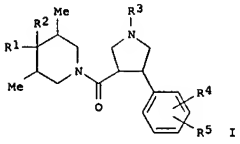
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005176772	A1	20050811	US 2005-51144	20050203
AU 2005213538	A1	20050825	AU 2005-213538	20050126
CA 2555800	A1	20050825	CA 2005-2555800	20050126
WO 2005077935	A1	20050825	WO 2005-IB208	20050126
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1716135	A1	20061102	EP 2005-702363	20050126
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU				
CN 1930146	A	20070314	CN 2005-80007573	20050126
NL 1028193	A1	20050808	NL 2005-1028193	20050204
NL 1028193	C2	20060420		
NO 2006003944	A	20061031	NO 2006-3944	20060904

PRIORITY APPLN. INFO.:

GB 2004-2492	A	20040204
US 2004-543950P	P	20040212
GB 2004-12417	A	20040603
US 2004-580209P	P	20040615
GB 2004-25530	A	20041119
US 2004-634916P	P	20041210
WO 2005-IB208	W	20050126

OTHER SOURCE(S): MARPAT 143:211844
GI

L4 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



I

AB The present invention relates to a class of melanocortin MCR4 agonists of general formula (I) wherein R1, R2, R3, R4 and R5 are as defined below and especially to selective MCR4 agonist compds., to their use in medicine, to compns. containing them, to processes for their preparation and to intermediates used in such processes. The variables for I are: R1 = optionally substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, alkylcycloalkyl, aryl, alkylaryl, heterocycle, or alkylheterocycle; R2 i= H, OH or OCH3; R3 = H, or optionally substituted alkyl, alkenyl,alkynyl, cycloalkyl, cycloalkenyl, alkylcycloalkyl, aryl, alkylaryl, heterocycle, or alkylheterocycle; R4 = H, alkyl, alkenyl,alkynyl, cycloalkyl, cycloalkenyl, halogen, (CH2)pOR6, (CH2)pNR7R8, CN, C(O)R6, C(O)OR6, C(O)NR7R8, (CH2)pNR7SO2R8, CF3, CH2CF3, OCF3 or OCH2CF3 wherein p=0, 1 or 2; R5 = alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, halogen, (CH2)pOR6, (CH2)pNR7R8, CN, C(O)R6, C(O)OR6, C(O)NR7R8, (CH2)pNR7SO2R8, CF3, CH2CF3, OCF3 or OCH2CF3 wherein p=0, 1 or 2; or R4 and R5 form a fused ring; R6, R7 and R8 = H, CH3 or CH2CH3. Compds. of the present invention are particularly suitable for treating female sexual dysfunction, male erectile dysfunction, obesity and diabetes.

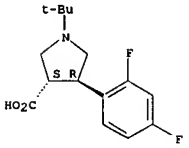
IT 455957-75-2P, (3S,4R)-1-tert-Butyl-4-(2,4-difluorophenyl)pyrrolidine-3-carboxylic acid hydrochloride
455957-94-5P, (3S,4R)-1-tert-Butyl-4-(2,4-difluorophenyl)pyrrolidine-3-carboxylic acid 862282-17-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of Pyrrolidinylcarbonyl piperidines as melanocortin receptor 4 agonists for therapeutic use)

RN 455957-75-2 CAPLUS

CN 3-Pyrrolidinecarboxylic acid, 4-(2,4-difluorophenyl)-1-(1,1-dimethylethyl)-, hydrochloride (1:1), (3S,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

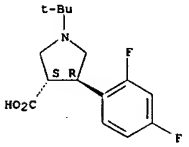
L4 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HCl

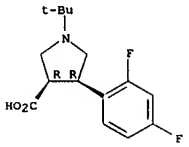
RN 455957-94-5 CAPLUS
CN 3-Pyrrolidinecarboxylic acid,
4-(2,4-difluorophenyl)-1-(1,1-dimethylethyl)-
, (3S,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 862282-17-5 CAPLUS
CN 3-Pyrrolidinecarboxylic acid,
4-(2,4-difluorophenyl)-1-(1,1-dimethylethyl)-
, (3R,4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

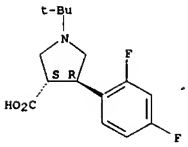


L4 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:283875 CAPLUS
DOCUMENT NUMBER: 143:7543
TITLE: Enantioselective Nitrile Anion Cyclization to Substituted Pyrrolidines. A Highly Efficient Synthesis of (3S,4R)-N-tert-Butyl-4-Arylpyrrolidine-3-Carboxylic Acid
AUTHOR(S): Chung, John Y. L.; Cvetovich, Raymond; Amato, Joseph; McWilliams, J. Christopher; Reamer, Robert; DiMichele, Lisa
CORPORATE SOURCE: Department of Process Research, Merck Research Laboratories, Rahway, NJ, 07065, USA
SOURCE: Journal of Organic Chemistry (2005), 70(9), 3592-3601
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:7543
AB A practical asym. synthesis of N-tert-Bu disubstituted pyrrolidines via a nitrile anion cyclization strategy is described. The five-step chromatog.-free synthesis of (3S,4R)-1-tert-butyl-4-(2,4-difluorophenyl)pyrrolidine-3-carboxylic acid from 2-chloro-1-(2,4-difluorophenyl)ethanone achieved a 71% overall yield. The cyclization substrate was prepared via a catalytic CBS asym. reduction, tert.-butylamine displacement of the chlorohydrin, and a conjugate addition of the hindered secondary amine to acrylonitrile. The key nitrile anion 5-exo-tet cyclization concomitantly formed the pyrrolidine ring with clean inversion of the C-4 center to afford 1,3,4-trisubstituted chiral pyrrolidine in >95% yield and 94-99% ee. Di-Et chlorophosphate and lithium hexamethyldisilazide were shown to be the resp. optimum activating group and base in this cyclization. The trans-cis mixture of the pyrrolidine nitrile undergoes a kinetically controlled epimerization/ saponification to afford the pure trans-pyrrolidine carboxylic acid target compound in >99.9% chemical and optical purity. This chemical was also shown to be applicable to both electronically neutral and rich substituted Ph substrates.
IT 455957-94-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (3S,4R)-N-tert-butyl-4-arylpyrrolidine-3-carboxylic acids by enantioselective nitrile anion cyclization)
RN 455957-94-5 CAPLUS
CN 3-Pyrrolidinecarboxylic acid,
4-(2,4-difluorophenyl)-1-(1,1-dimethylethyl)-
, (3S,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

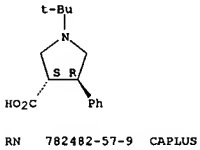
L4 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L4 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



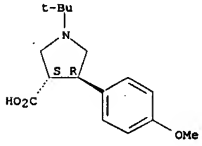
IT 782482-56-8P 782482-57-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (3S,4R)-N-tert-butyl-4-arylpyrrolidine-3-carboxylic acids by enantioselective nitrile anion cyclization)
RN 782482-56-8 CAPLUS
CN 3-Pyrrolidinecarboxylic acid, 1-(1,1-dimethylethyl)-4-phenyl-, (3S,4R)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 782482-57-9 CAPLUS
CN 3-Pyrrolidinecarboxylic acid, 1-(1,1-dimethylethyl)-4-(4-methoxyphenyl)-,
(3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

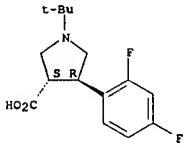
L4 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:902344 CAPLUS
DOCUMENT NUMBER: 141:379798
TITLE: A process for preparation of pyrrolidinecarboxylic acid derivatives, useful for treatment of melanocortin receptor mediated diseases
INVENTOR(S): Cvetovich, Raymond; Chung, John Y.; Amato, Joseph S.; Dimichele, Lisa
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

Instant App

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004092126	A2	20041028	WO 2004-US11253	20040409
WO 2004092126	A3	20050120		
WO 2004092126	B1	20050331		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2521487	A1	20041028	CA 2004-2521487	20040409
EP 1615882	A2	20060118	EP 2004-750027	20040409
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
CN 1774419	A	20060517	CN 2004-80009882	20040409
JP 2006523700	T	20061019	JP 2006-509940	20040409
US 2006199958	A1	20060907	US 2005-550640	20050923
PRIORITY APPLN. INFO.:			US 2003-462795P	P 20030414
			WO 2004-US11253	W 20040409

OTHER SOURCE(S): CASREACT 141:379798; MARPAT 141:379798
GI

L4 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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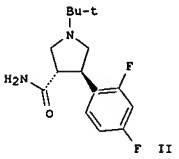
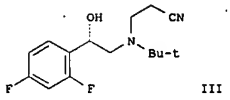


II



III

AB The invention relates to a preparation of pyrrolidinecarboxylic acid derivs. of formula I [wherein: R1 is H, NH2, alkyl, or (CH2)0-4-heteroaryl, etc.; R2 is (cyclo)alkyl, furyl, oxazolyl, or thienyl, etc.]. These compds. are useful for treatment of melanocortin receptor mediated diseases such as obesity, diabetes, male sexual dysfunction, and female sexual dysfunction (no biol. data). For instance, pyrrolidinecarboxylic acid derivative II was prepared via intramol. heterocyclization of the obtained amine III and hydrolysis (example 1).

IT 455957-94-5P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for preparation of pyrrolidinecarboxylic acid derivs. useful for treatment of melanocortin receptor mediated diseases)

RN 455957-94-5 CAPLUS
CN 3-Pyrrolidinecarboxylic acid, 4-(2,4-difluorophenyl)-1-(1,1-dimethylethyl)-, (3S,4R)- (CA INDEX NAME)

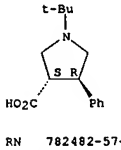
Absolute stereochemistry. Rotation (-).

L4 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

IT 782482-56-8P 782482-57-9P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(process for preparation of pyrrolidinecarboxylic acid derivs. useful for treatment of melanocortin receptor mediated diseases)

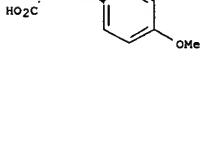
RN 782482-56-8 CAPLUS
CN 3-Pyrrolidinecarboxylic acid, 1-(1,1-dimethylethyl)-4-phenyl-, (3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 782482-57-9 CAPLUS
CN 3-Pyrrolidinecarboxylic acid, 1-(1,1-dimethylethyl)-4-(4-methoxyphenyl)-, (3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:872662 CAPLUS
DOCUMENT NUMBER: 141:366128
TITLE: Preparation of cycloalkylcarbonyl or heterocycloalkylcarbonyl-substituted spiropiperidines as melanocortin-4 receptor agonists for the treatment of conditions such as obesity
INVENTOR(S): Guo, Liangqin; He, Shuwen; Jian, Tianying; Lai, Yingjie; Liu, Jian; Nargund, Ravi P.; Sebhat, Iyassu K.; Ujjainwalla, Feroze; Ye, Zhixiong; Young, Jonathan R.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 200 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004089307	A2	20041021	WO 2004-US9751	20040331
WO 2004089307	A3	20050331		
WO 2004089307	A8	20050623		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004227835	A1	20041021	AU 2004-227835	20040331
CA 2520114	A1	20041021	CA 2004-2520114	20040331
EP 1613601	A2	20060111	EP 2004-749540	20040331
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
BR 2004009078	A	20060418	BR 2004-9078	20040331
CN 1768041	A	20060503	CN 2004-80009148	20040331
JP 2006522132	T	20060928	JP 2006-509489	20040331
JP 3856815	B2	20061213		
US 2006183904	A1	20060817	US 2005-548350	20050907
NO 2005005166	A	20051230	NO 2005-5166	20051103
PRIORITY APPLN. INFO.:			US 2003-460293P	P 20030404
			WO 2004-US9751	W 20040331

OTHER SOURCE(S): MARPAT 141:366128
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I or II (X,Y = R62C, R9N, C(:O); Y,X = R62C, R6N, C(:O),

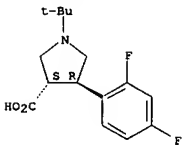
L4 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
R6N:C, O, S, S(:O), SO2; XY = CR6:CR6; Z = R1C, N; A = (CH2)m; E = (CH2)p;
R1 = H, amidino, (un)substituted aminoalkyl, iminoylalkyl, alkyl, cycloalkylalkyl, phenylalkyl, naphthylalkyl, or heteroarylalkyl; R2 = (un)substituted Ph, naphthyl, heteroaryl; R4 = H, (un)substituted alkyl, halogen, alkoxy, O2N, F3C, F3CCH2, F3CO, F3CCH2O; R6, R9 = H, (un)substituted alkyl, phenylalkyl, naphthylalkyl, heteroarylalkyl, cycloalkylalkyl, heterocycloalkylalkyl, aminoalkyl, carboxyalkyl, etc.; m, p = 1, 2; n = 0-3] such as III•HCl are prepd. as melanocortin-4 receptor agonists for the treatment of obesity and related conditions such as diabetes, bulimia, insulin resistance, and hyperlipidemia; a variety of other conditions, particularly male and female sexual dysfunction and erectile dysfunction, are also potentially treatable with the title compds. Oxoindanospiropiperidinecarboxylate IV is reduced with sodium borohydride and the alc. eliminated in the presence of p-toluenesulfonic acid to give the indenespiropiperidinecarboxylate; Jacobsen epoxidn. of the indene double bond, opening of the epoxide with sodium azide, aziridine formation using a fluorous phosphine, N-methylation of the aziridine, regioselective redn. of the aziridine with sodium borohydride to yield the aminoindanospiropiperidinecarboxylate, acylation with 2-acetoxyisobutyryl chloride, hydrolysis of the ester with sodium methoxide and methylation of the alc. with Me iodide, deprotection of the piperidine nitrogen, and acylation with nonracemic trans-4-(2,4-difluorophenyl)-1-tert-butyl-3-pyrrolidinecarboxylic acid yields III. Some of the title compds. bind to the melanocortin-4 receptor with IC50 values of <10 μM and <5 μM (no data).

IT 455957-75-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of cycloalkylcarbonyl or heterocycloalkylcarbonyl-substituted spiropiperidines as melanocortin-4 receptor agonists for the treatment of conditions such as obesity and male or female sexual dysfunction)

RN 455957-75-2 CAPLUS
CN 3-Pyrrolidinecarboxylic acid, 4-(2,4-difluorophenyl)-1-(1,1-dimethylethyl)-, hydrochloride (1:1), (3S,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L4 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



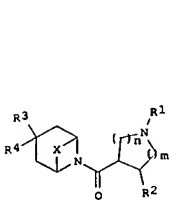
● HCl

L4 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:857404 CAPLUS
DOCUMENT NUMBER: 141:350043
TITLE: Preparation of bicyclic piperidine derivatives as melanocortin-4 receptor agonists
INVENTOR(S): Nargund, Ravi P.; Ye, Zhixiong; Guo, Liangqin
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 103 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004087159	A1	20041014	WO 2004-US8711	20040322
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004226452	A1	20041014	AU 2004-226452	20040322
CA 2519939	A1	20041014	CA 2004-2519939	20040322
EP 1610789	A1	20060104	EP 2004-758182	20040322
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK				
CN 1764458	A	20060426	CN 2004-80008218	20040322
JP 2006521359	T	20060921	JP 2006-507449	20040322
US 2006194780	A1	20060831	US 2005-548782	20050912
PRIORITY APPLN. INFO.:			US 2003-457679P	P 20030326
			WO 2004-US8711	A 20040322

OTHER SOURCE(S): MARPAT 141:350043
GI



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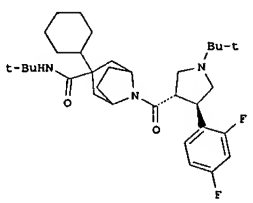


II

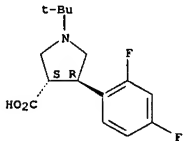
L4 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

AB Title compds. I (R1 = H, amidino, alkyl, (un)substituted-arylalkyl, etc.; R2 = alkyl, (un)substituted-Ph, -naphthyl, and -heteroaryl; R3 and R4 independently = H, alkyl, alkenyl, cyanoalkyl, etc.; X = (CR5R6)p wherein R5 and R6 independently = H, alkyl, OH, amino, halo, cycloalkylalkyl, etc. and p = 1-3; m = 0-2; n = 1-2) are prepared and disclosed as agonists of the human melanocortin receptor(s) and, in particular, are selective agonists of the human melanocortin-4 receptor (MC-4R). Thus, e.g., II was prepared in a multistep synthesis from N-carbethoxy-4-tropinone to provide 3-[(tert-butylamino)carbonyl]-3-cyclohexyl-8-azabicyclo[3.2.1]octane which was amidated with (3R,4S)-1-tert-butyl-4-(2,4-difluorophenyl)pyrrolidine-3-carboxylic acid (preparation given). Representative compds. of the invention were tested and found to bind to the melanocortin-4 receptor and possessed IC50 values less than 10 μM. They are therefore useful for the treatment, control, or prevention of diseases and disorders responsive to the activation of MC-4R, such as obesity, diabetes, sexual dysfunction, including erectile dysfunction and female sexual dysfunction.

IT 455957-94-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of bicyclic piperidine derivs. as melanocortin-4 receptor agonists)

RN 455957-94-5 CAPLUS
CN 3-Pyrrolidinecarboxylic acid, 4-(2,4-difluorophenyl)-1-(1,1-dimethylethyl)-, (3S,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



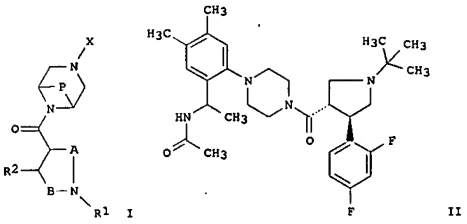
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:756685 CAPLUS
DOCUMENT NUMBER: 141:277640
TITLE: Preparation of acylated piperazine derivatives as melanocortin -4 receptor agonists for the treatment of obesity, diabetes mellitus and sexual dysfunction, and pharmaceutical compositions thereof
INVENTOR(S): Bakshi, Raman K.; Guo, Liangqin; Hong, Qingmei; Nargund, Ravi P.; Pollard, Patrick G.; Sebhat, Iyassu K.; Ujjainwalla, Feroze; Ye, Zhixiong
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 187 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004078717	A1	20040916	WO 2004-US7713	20040227
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004204398	A1	20041014	US 2004-788859	20040227
US 7160886	B2	20070109		
PRIORITY APPLN. INFO.:			US 2003-451502P P	20030303
			US 2003-515943P P	20031030

OTHER SOURCE(S): MARPAT 141:277640
GI

L4 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



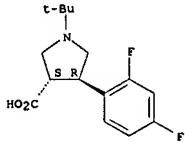
I II

AB N-Acylated piperazine derivs. of formula I, wherein X is (un)substituted alkyl/phenyl/heteroaryl, etc.; R1 is H, amidino, (un)substituted (cyclo)alkyl/alkyliminoyl/phenyl/naphthyl/heteroaryl, etc.; R2 is (un)substituted phenyl/naphthyl/heteroaryl; P is (CHR4R4)m; R4 is H, (cyclo)alkyl(alkyl), aryl(alkyl), OH, halo, amino; m is 0-4; A is (CH2)r; r is 1 or 2; B = (CH2)s; s is 0-2, were prepared as melanocortin-4 receptor (MC-4R) agonists. II is one of the given examples, which was synthesized in several steps via coupling of the corresponding monosubstituted piperazine (preparation given) with the corresponding pyrrolidinecarboxylic acid (preparation given). Compds. I, including some specific stereoisomers, pharmaceutically acceptable salts thereof, and pharmaceutical compns. (examples given) comprising I and pharmaceutically acceptable carriers, are claimed. Certain compds. among I are agonists of the human melanocortin receptor(s) and, in particular, are selective agonists of the human MC-4R. Representative compds. (no indication) were tested and found to bind to the melanocortin-4 receptor, generally having IC50 values less than 10 μM. Representative compds. (no indication) were also tested in the functional model assay, and found generally to activate the MC-4R with EC50 values less than 10 μM. Compds. I are therefore useful for the treatment, control, or prevention of diseases and disorders responsive to the activation of MC-4R, such as obesity, diabetes, sexual dysfunction, including erectile dysfunction and female sexual dysfunction.

IT 455957-94-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of phenylpyrrolidinylcarbonyl/phenylpiperidinylcarbonyl piperazines as melanocortin-4 receptor agonists)
RN 455957-94-5 CAPLUS
CN 3-Pyrrolidinecarboxylic acid, 4-(2,4-difluorophenyl)-1-(1,1-dimethylethyl)-

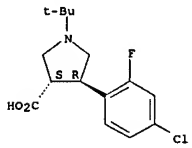
L4 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
, (3S,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 757974-04-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; preparation of phenylpyrrolidinylcarbonyl/phenylpiperidinylcarbonyl piperazines as melanocortin-4 receptor agonists)
RN 757974-04-2 CAPLUS
CN 3-Pyrrolidinecarboxylic acid, 4-(4-chloro-2-fluorophenyl)-1-(1,1-dimethylethyl)-, (3S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

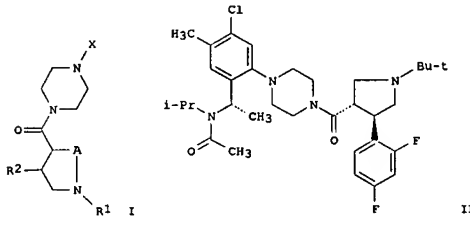


REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L4 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:756684 CAPLUS
DOCUMENT NUMBER: 141:277639
TITLE: Preparation of acylated piperazine derivatives as melanocortin-4 receptor agonists for the treatment of obesity, diabetes mellitus and sexual dysfunction, and pharmaceutical compositions thereof
INVENTOR(S): Bakshi, Raman K.; Hong, Qingmei; Nargund, Ravi P.; Pollard, Patrick G.; Sebhat, Iyassu K.; Ujjainwalla, Feroze; Ye, Zhixiong
PATENT ASSIGNEE(S): Merck & Co. Inc., USA
SOURCE: PCT Int. Appl., 76 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004078716	A1	20040916	WO 2004-US5982	20040227
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004204398	A1	20041014	US 2004-788859	20040227
US 7160886	B2	20070109		
PRIORITY APPLN. INFO.:			US 2003-451502P P	20030303
			US 2003-515943P P	20031030

OTHER SOURCE(S): MARPAT 141:277639
GI



I II

L4 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

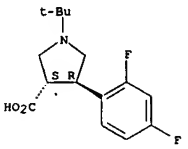
AB N-Acylated piperazine derivs. of formula I, wherein X is (un)substituted alkyl/phenyl/phenylalkyl; R1 is alkyl; R2 is (un)substituted phenyl; A is (CH2)r; r is 1 or 2, were prepared as melanocortin-4 receptor (MC-4R) agonists. II is one of the given examples, which was synthesized in several steps via coupling of the left part, a phenylpiperazine (preparation given), with the right part, a phenylpyrrolidinecarboxylic acid (preparation given). Compds. I and pharmaceutically acceptable salts thereof as well as pharmaceutical compns. (examples given) comprising I and pharmaceutically acceptable carriers are claimed. Representative compds. (no indication) were tested and found to bind to the melanocortin-4 receptor, generally having IC50 values less than 10 μM. Representative compds. (no indication) were also examined in several functional model tests, and found generally able to activate the MC-4R with EC50 values less than 10 μM. Certain compds. are agonists of the human melanocortin receptor(s) and, in particular, are selective agonists of the human MC-4R. They are therefore useful for the treatment, control, or prevention of diseases and disorders responsive to the activation of MC-4R, such as obesity, diabetes, sexual dysfunction, including erectile dysfunction and female sexual dysfunction.

IT 455957-94-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of acylated piperazine derivs. as melanocortin-4 receptor agonists)

RN 455957-94-5 CAPLUS

CN 3-Pyrrolidinecarboxylic acid, 4-(2,4-difluorophenyl)-1-(1,1-dimethylethyl)-, (3S,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:675993 CAPLUS
DOCUMENT NUMBER: 137:216874
TITLE: Acylated piperidine derivatives, specifically 1-(pyrrolidinylcarbonyl)piperidines, 1-(piperidinylcarbonyl)piperidines, and analogs, as melanocortin-4 receptor agonists, and their pharmaceutical compositions and therapeutic uses
INVENTOR(S): Ujjainwalla, Feroze; Chu, Lin; Goulet, Mark T.; Lee, Bonnie; Warner, Daniel; Wyvratt, Matthew J.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 112 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002068388	A2	20020906	WO 2002-US5724	20020225
WO 2002068388	A3	20030313		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2439152	A1	20020906	CA 2002-2439152	20020225
AU 2002258414	A1	20020912	AU 2002-258414	20020225
EE 200300415	A	20031215	EE 2003-415	20020225
EP 1383501	A2	20040128	EP 2002-728357	20020225
EP 1383501	B1	20070404		
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HU 200303376	A2	20040128	HU 2003-3376	20020225
JP 2004529105	T	20040924	JP 2002-567902	20020225
NZ 527364	A	20041224	NZ 2002-527364	20020225
CN 1633297	A	20050629	CN 2002-805674	20020225
BR 2002007658	A	20051025	BR 2002-7658	20020225
AT 358481	T	20070415	AT 2002-728357	20020225
US 2003225060	A1	20031204	US 2003-356879	20030203
US 6818658	B2	20041116		
ZA 2003006160	A	20040721	ZA 2003-6160	20030808
BG 108132	A	20041230	BG 2003-108132	20030825
IN 2003CN01342	A	20051125	IN 2003-CN1342	20030826
NO 2003003812	A	20031028	NO 2003-3812	20030827
US 2004266821	A1	20041230	US 2004-894719	20040720

PRIORITY APPLN. INFO.: US 2001-272258P P 20010228
US 2001-300118P P 20010622
WO 2002-US5724 W 20020225

L4 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
US 2003-356897 A3 20030203

OTHER SOURCE(S): MARPAT 137:216874
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Certain novel 4-substituted N-acylated piperidine derivs., specifically I, are agonists of the human melanocortin receptor(s) and, in particular, are selective agonists of the human melanocortin-4 receptor (MC-4R) [wherein: p = 1 or 2; q = 0, 1, or 2; n = 0, 1, or 2; R1 = H, amidino, alkyliminoyl, (un)substituted alkyl, (CH2)n-G1 [G1 = (un)substituted cycloalkyl, Ph, naphthyl, or heteroaryl]; R2 = (un)substituted Ph, naphthyl, or heteroaryl; X = alkyl, (CH2)n-G2 [G2 = (un)substituted cycloalkyl, Ph, naphthyl, heteroaryl, heterocyclyl, cyano, CONH2, CO2H, OH, NH2, and various derivs.] where any of (CH2)n may also be substituted; including pharmaceutically acceptable salts]. They are therefore useful for the treatment, control, or prevention of diseases and disorders responsive to the activation of MC-4R, such as obesity, diabetes, sexual dysfunction, including erectile dysfunction and female sexual dysfunction. Approx. 180 invention compds. I and approx. 25 intermediates were prepared For instance, (2-bromo-5-chlorophenyl)acetic acid underwent a sequence of Me esterification, coupling with tert-Bu 4-[[(trifluoromethyl)sulfonyl]oxy]-3,6-dihydropyridine-1(2H)-carboxylate via a boronate ester, removal of the BOC group, and amidation with (3S,4R)-1-(tert-butyl)-4-(2,4-difluorophenyl)pyrrolidine-3-carboxylic acid. The unsatd. amide-ester underwent hydrogenation, saponification of the ester, and amidation with MeNH2.HCl, to give title compound II. Representative compds. I bound to cloned human MC-4R in vitro with IC50 values generally below 2 μM, and also acted as agonists toward cloned human MCR in a functional assay with EC50 values less than 1 μM.

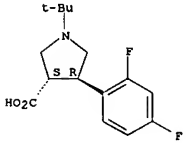
IT 455957-75-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of acylated piperidine derivs., particularly (pyrrolidinylcarbonyl)piperidines, (piperidinylcarbonyl)piperidines, and analogs, as melanocortin-4 receptor agonists)

RN 455957-75-2 CAPLUS

CN 3-Pyrrolidinecarboxylic acid, 4-(2,4-difluorophenyl)-1-(1,1-dimethylethyl)-, hydrochloride (1:1), (3S,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L4 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



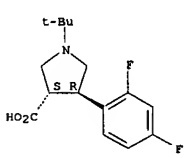
● HCl

IT 455957-94-5, (3S,4R)-1-tert-Butyl-4-(2,4-difluorophenyl)pyrrolidine-3-carboxylic acid 455957-95-6, (3R,4S)-1-tert-Butyl-4-(2,4-difluorophenyl)pyrrolidine-3-carboxylic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(precursor; preparation of acylated piperidine derivs., particularly (pyrrolidinylcarbonyl)piperidines, (piperidinylcarbonyl)piperidines, and analogs, as melanocortin-4 receptor agonists)

RN 455957-94-5 CAPLUS

CN 3-Pyrrolidinecarboxylic acid, 4-(2,4-difluorophenyl)-1-(1,1-dimethylethyl)-, (3S,4R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

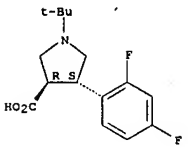


RN 455957-95-6 CAPLUS

CN 3-Pyrrolidinecarboxylic acid, 4-(2,4-difluorophenyl)-1-(1,1-dimethylethyl)-, (3R,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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NEWS 4	JAN 16	IPC version 2007.01 thesaurus available on STN
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NEWS 22	MAR 30	RDISCLOSURE reloaded with enhancements
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NEWS 29	MAY 08	CA/CAplus Indian patent publication number format defined
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NEWS 32	MAY 21	TOXCENTER enhanced with BIOSIS reload
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FILE CONTENT:1840 - 27 May 2007 VOL 146 ISS 23

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Uploading C:\Program Files\Stnexp\Queries\10550640\3.str
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chain nodes :
7 8 9 10 11 12 13 14 16 17
ring nodes :
1 2 3 4 5
chain bonds :
1-8 2-7 9-10 9-12 10-11 11-16 11-17 12-13 13-14
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-8 2-3 2-7 3-4 4-5 9-10 9-12 11-16 11-17 13-14
exact bonds :
10-11 12-13

G1:CO2H,COOH,CN

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 16:CLASS 17:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
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node mappings:
2:13 3:12 4:9 5:10 1:11

L1 STRUCTURE UPLOADED

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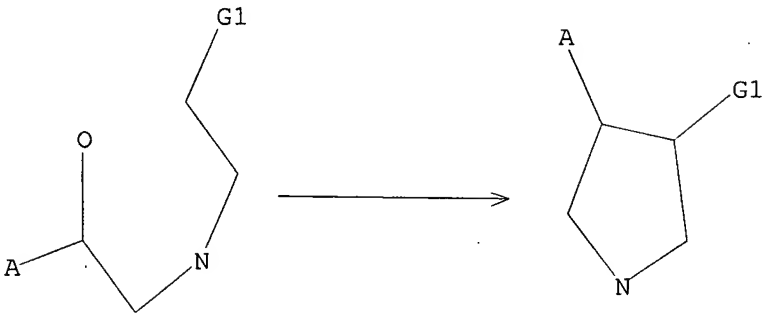
L1 HAS NO ANSWERS
L1 STR



G1 CO2H,COOH,CN

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 10:47:40 FILE 'CASREACT'
SCREENING COMPLETE - 6 REACTIONS TO VERIFY FROM 4 DOCUMENTS

100.0% DONE 6 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED VERIFICATIONS: 6 TO 266
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1 (0 REACTIONS)

=> s l1 full
FULL SEARCH INITIATED 10:47:47 FILE 'CASREACT'
SCREENING COMPLETE - 890 REACTIONS TO VERIFY FROM 126 DOCUMENTS

100.0% DONE 890 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1 (0 REACTIONS)

=>

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